

PREDICTION OF STEADY STATE FLOW IN RANDOMLY HETEROGENEOUS FORMATIONS BY CONDITIONAL NONLOCAL FINITE ELEMENTS

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Abstract

We consider the effect of measuring randomly varying hydraulic conductivity $K(\mathbf{x})$ on one's ability to predict deterministically, without any upscaling, two-dimensional steady state flow subject to random sources and/or boundary conditions. Such prediction is possible by means of first ensemble moments of heads and fluxes, conditioned on measured values of $K(\mathbf{x})$; the uncertainty associated with such prediction can be quantified by means of the corresponding conditional second moments. As these predictors vary generally more smoothly over space than their random counterparts, they are resolved on coarser grids without upscaling by nonlocal Galerkin finite elements. We compare the head and flux predictions resulted from using two methodologies of inferring conditional ensemble moments of $K(\mathbf{x})$ from available data. The first approach relies on the *known* statistical distribution of $K(\mathbf{x})$ to generate conditional (thus non-stationary) fields of the natural log-hydraulic conductivity $Y(\mathbf{x}) = \ln K(\mathbf{x})$ with prescribed mean and variance. In the second approach, the experimental measurements of Y at selected locations are used (by means of kriging) to estimate $Y(\mathbf{x})$ at points where it is not known, and to evaluate autocovariance of estimation error associated with such a prediction. The results obtained from both approaches are compared with conditional Monte Carlo simulation (MCS). Our nonlocal finite element solution based on the first approach is in excellent agreement with MCS. The finite element solution based on the kriging estimates smoothes spatial variability of the unbiased head and flux predictors, and their covariances.

1. Introduction

Accurate prediction of hydraulic head, $h(\mathbf{x})$, and specific discharge, $\mathbf{q}(\mathbf{x})$, in

geological formations is an extremely difficult task due to lack of information about heterogeneity and unprecise measurements. As a consequence, porous media properties can be modeled as random space functions and flow and transport problems can be treated stochastically (Dagan and Neuman, 1997). We consider steady state groundwater flow governed by

$$-\nabla \cdot \mathbf{q}(\mathbf{x}) + f(\mathbf{x}) = 0; \quad \mathbf{q}(\mathbf{x}) = -\mathbf{K}(\mathbf{x}) \nabla h(\mathbf{x}); \quad \mathbf{x} \in \Omega \quad (1)$$

$$h(\mathbf{x}) = H(\mathbf{x}), \quad \mathbf{x} \in \Gamma_D; \quad -\mathbf{q}(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) = Q(\mathbf{x}), \quad \mathbf{x} \in \Gamma_N \quad (2)$$

where $f(\mathbf{x})$ is a randomly prescribed source term, $H(\mathbf{x})$ is a randomly prescribed head on Dirichlet boundary Γ_D , $Q(\mathbf{x})$ is a randomly prescribed flux into flow domain Ω across Neumann boundary Γ_N , and $\mathbf{n}(\mathbf{x})$ is a unit outward normal to the boundary $\Gamma = \Gamma_D \cup \Gamma_N$. The forcing terms $f(\mathbf{x})$, $H(\mathbf{x})$ and $Q(\mathbf{x})$ are prescribed in a statistically independent manner at the same scale as $\mathbf{q}(\mathbf{x})$, $\mathbf{K}(\mathbf{x})$ and $h(\mathbf{x})$. As the hydraulic conductivity $\mathbf{K}(\mathbf{x})$ and forcing functions are random, (1) – (2) constitute a system of stochastic partial differential equations.

In general, averaging (1) – (2) analytically requires adopting simplifying assumptions such as treating the natural log hydraulic conductivity $Y(\mathbf{x}) = \ln \mathbf{K}(\mathbf{x})$ to a statistically homogeneous Gaussian field with a small variance $\sigma_Y^2 \ll 1$. Analytical solutions of heads and fluxes moments are usually obtained to second-order in σ_Y in conjunction with the infinite domain hypothesis (e.g. Dagan and Neuman, 1997, and references therein). The analytical approach can not easily accommodate the influence of boundaries (e.g. Tartakovsky and Neuman, 1998b) and the effect of conditioning points. To overcome some of these difficulties, the numerical Monte Carlo method has been adopted to solve the groundwater flow (e.g. Naff *et al.*, 1998, and references therein). A powerful alternative to these approaches is the exact nonlocal formalism for the prediction of flow in randomly heterogeneous porous media by conditional moments, proposed by Neuman and coworkers (Neuman and Orr, 1993; Neuman *et al.*, 1996; Guadagnini and Neuman, 1997, 1998; Tartakovsky and Neuman, 1998a). Their theoretical framework allows deriving exact conditional first and second moment equations, which formally include boundaries with random conditions, random source terms, and hydraulic conductivity conditioning points. Recursive closure approximations for the moment equations of flow were developed for steady and unsteady state flow. They are based on an expansion in powers of σ_Y , which represents the standard estimation error of (natural) log hydraulic conductivity. For steady state flow, Guadagnini and Neuman (1997, 1998) developed finite elements algorithms for computing the first and second conditional statistical moments of $h(\mathbf{x})$ and $\mathbf{q}(\mathbf{x})$ to first order in σ_Y^2 . They analyzed two-dimensional non-uniform flow towards a pumping well in weakly and strongly heterogeneous hydraulic conductivity fields conditioned on measured values at several points. Their results were in excellent agreement with numerical Monte Carlo simulations. The authors recognized that a crucial point in assessing the applicability of their methodology to real world problems is the development of a reliable methodology to infer estimates of spatial distribution of $\mathbf{K}(\mathbf{x})$ and covariance structure of associated prediction error on the basis of available field data.

In this paper we consider two methodologies for this purpose: (a) synthetic generation and ensemble averaging of conditional (thus non-stationary) fields of the natural log-hydraulic conductivity $Y(\mathbf{x}) = \ln K(\mathbf{x})$ with prescribed mean and variance; (b) kriging estimation of desired quantities. We assume that $K(\mathbf{x})$ has been determined (without measurement errors) at selected locations by standard methods, such as pumping. We further assume that it is possible to infer the conditional unbiased estimates of hydraulic conductivities (in particular their conditional mean values, $\langle K(\mathbf{x}) \rangle_c$), and the spatial auto-covariance of the associated random estimation errors $K'(\mathbf{x}) = K(\mathbf{x}) - \langle K(\mathbf{x}) \rangle_c$ from discrete measurements of $K(\mathbf{x})$. We then solve the nonlocal moment equations by finite elements on a rectangular grid in two dimensions by means of the Finite Elements methodology introduced by Guadagnini and Neuman (1997, 1998) and compare results with those obtained by solving the original flow problem by conditional Monte Carlo simulation.

2. Equations for Conditional Moments

The optimum unbiased flux and head predictors, $\langle \mathbf{q}(\mathbf{x}) \rangle_c$ and $\langle h(\mathbf{x}) \rangle_c$, have been shown (Neuman and Orr, 1993; Neuman *et al.*, 1996; Guadagnini and Neuman, 1997) to satisfy up to second order in σ_Y the following boundary value problem

$$\nabla \cdot \left[K_G(\mathbf{x}) \nabla \langle h^{(0)}(\mathbf{x}) \rangle_c \right] + \langle f(\mathbf{x}) \rangle = 0 \quad \mathbf{x} \in \Omega \quad (3)$$

$$\langle h^{(0)}(\mathbf{x}) \rangle_c = \langle H(\mathbf{x}) \rangle \quad \mathbf{x} \in \Gamma_D \quad (4)$$

$$K_G(\mathbf{x}) \nabla \langle h^{(0)}(\mathbf{x}) \rangle_c \cdot \mathbf{n}(\mathbf{x}) = \langle Q(\mathbf{x}) \rangle \quad \mathbf{x} \in \Gamma_N \quad (5)$$

$$\nabla \cdot \left[K_G(\mathbf{x}) \left(\nabla \langle h^{(2)}(\mathbf{x}) \rangle_c + \frac{\sigma_Y^2(\mathbf{x})}{2} \nabla \langle h^{(0)}(\mathbf{x}) \rangle_c \right) - \mathbf{r}_c^{(2)}(\mathbf{x}) \right] = 0 \quad \mathbf{x} \in \Omega \quad (6)$$

$$\langle h^{(2)}(\mathbf{x}) \rangle_c = 0 \quad \mathbf{x} \in \Gamma_D \quad (7)$$

$$\left[K_G(\mathbf{x}) \left(\nabla \langle h^{(2)}(\mathbf{x}) \rangle_c + \frac{\sigma_Y^2(\mathbf{x})}{2} \nabla \langle h^{(0)}(\mathbf{x}) \rangle_c \right) - \mathbf{r}_c^{(2)}(\mathbf{x}) \right] \cdot \mathbf{n}(\mathbf{x}) = 0 \quad \mathbf{x} \in \Gamma_N \quad (8)$$

where $\langle h^{(i)}(\mathbf{x}) \rangle_c$ is i -th order approximations of head predictors, and K_G is the conditional geometric mean of K . Here

$$\mathbf{r}_c^{(2)}(\mathbf{x}) = \int_{\Omega} \mathbf{a}_c^{(2)}(\mathbf{y}, \mathbf{x}) \nabla_y \langle h^{(0)}(\mathbf{y}) \rangle_c d\mathbf{y} \quad (9)$$

$$\mathbf{a}_c^{(2)}(\mathbf{y}, \mathbf{x}) = K_G(\mathbf{x}) K_G(\mathbf{y}) C_{Yc}(\mathbf{x}, \mathbf{y}) \nabla_x \nabla_y^T \langle G^{(0)}(\mathbf{y}, \mathbf{x}) \rangle_c \quad (10)$$

$\langle G^{(0)} \rangle_c$ is a zeroth-order Green's function and $C_{Yc}(\mathbf{x}, \mathbf{y}) = \langle Y'(\mathbf{x}) Y'(\mathbf{y}) \rangle_c$ is the conditional auto-covariance of Y . The second-order flux approximation is nonlocal and non-Darcian.

With zero-variance forcing terms, the second-order approximation of the conditional covariance of hydraulic head prediction, $C_{hc}(\mathbf{x}, \mathbf{y}) = \langle h'(\mathbf{x}) h'(\mathbf{y}) \rangle_c$, satisfies (Guadagnini and Neuman, 1997)

$$\nabla_x \cdot \left[\mathbf{K}_G(\mathbf{x}) \nabla_x C_{hc}^{(2)}(\mathbf{x}, \mathbf{y}) + C_{hKc}^{(2)}(\mathbf{x}, \mathbf{y}) \nabla_x \langle h^{(0)}(\mathbf{x}) \rangle_c \right] = 0 \quad \mathbf{x} \in \Omega \quad (11)$$

$$C_{hc}^{(2)}(\mathbf{x}, \mathbf{y}) = 0 \quad \mathbf{x} \in \Gamma_D \quad (12)$$

$$\left[\mathbf{K}_G(\mathbf{x}) \nabla_x C_{hc}^{(2)}(\mathbf{x}, \mathbf{y}) + C_{hKc}^{(2)}(\mathbf{x}, \mathbf{y}) \nabla_x \langle h^{(0)}(\mathbf{x}) \rangle_c \right] \cdot \mathbf{n}(\mathbf{x}) = 0 \quad \mathbf{x} \in \Gamma_N \quad (13)$$

where second-order approximation of $C_{hKc}(\mathbf{x}, \mathbf{y}) = \langle h'(\mathbf{x}) K'(\mathbf{y}) \rangle_c$, is given by

$$C_{hKc}^{(2)}(\mathbf{x}, \mathbf{y}) = -\mathbf{K}'_G(\mathbf{x}) \int_{\Omega} \nabla_z \langle h^{(0)}(\mathbf{z}) \rangle_c \cdot \nabla_z \langle G^{(0)}(\mathbf{z}, \mathbf{y}) \rangle_c \mathbf{K}'_G(\mathbf{z}) C_{Yc}(\mathbf{z}, \mathbf{x}) dz \quad (14)$$

Second-order approximation of the conditional flux covariance tensor $C_{qc}(\mathbf{x}, \mathbf{y}) = \langle \mathbf{q}'(\mathbf{x}) \mathbf{q}'(\mathbf{y})^T \rangle_c$ is given by

$$\begin{aligned} C_{qc}^{(2)}(\mathbf{x}, \mathbf{y}) = & \mathbf{K}_G(\mathbf{x}) \mathbf{K}_G(\mathbf{y}) \left[\nabla_x \nabla_y^T C_{hc}^{(2)}(\mathbf{x}, \mathbf{y}) \right. \\ & + C_{Yc}(\mathbf{x}, \mathbf{y}) \nabla_x \langle h^{(0)}(\mathbf{x}) \rangle_c \nabla_y^T \langle h^{(0)}(\mathbf{y}) \rangle_c \left. \right] \\ & + \mathbf{K}_G(\mathbf{y}) \nabla_x \langle h^{(0)}(\mathbf{x}) \rangle_c \nabla_y^T C_{hKc}^{(2)}(\mathbf{x}, \mathbf{y}) \\ & + \mathbf{K}_G(\mathbf{x}) \nabla_x C_{hKc}^{(2)}(\mathbf{y}, \mathbf{x}) \nabla_y^T \langle h^{(0)}(\mathbf{y}) \rangle_c \end{aligned} \quad (15)$$

Equations (3) – (15) constitute a closed system of equations with statistical moments of Y serving as input parameters. In what follows, we explore two alternatives to evaluating these moments, and their influence on the solution of (3) – (15).

3. Computational Procedure and Examples

To compute the conditional moments of $Y(\mathbf{x})$ from the available data, we employ two methodologies. The first methodology utilizes the prescribed ("known" *a priori*) probability density function to generate a set of conditional, and thus non-stationary, random fields (realizations) of $Y(\mathbf{x})$ with given conditional mean $\langle Y(\mathbf{x}) \rangle_c$ and autocovariance function $C_{Yc}(\mathbf{x}, \mathbf{y})$. In our simulations we generated $NMC = 1000$ of such realizations using the Gaussian sequential simulator GCOSIM of Gomez Hernandez (1991). The second methodology treats $\langle Y(\mathbf{x}) \rangle_c$ as a kriging estimate and computes the corresponding

autocovariance of estimation errors by kriging equations. The first approach appears to be more theoretically sound since it relies on the well established Law of Large Numbers to prove the ergodicity hypothesis. It is also a methodology most widely used in the current literature on stochastic analysis of groundwater flow and transport. The second approach has more of a practical value, since in reality one has but a limited number of experimental data to work with. The main purpose of this study is to compare both approaches with the aim to obtain the best prediction of the hydraulic head and flux distributions. To meet this goal, we solve the moments equations (3) – (15) by Galerkin finite elements (computational details are described by Guadagnini and Neuman, 1997) on a rectangular grid with $M = 3600$ square elements (40 rows by 90 columns) of uniform size $\Delta x_1 = \Delta x_2 = 0.2$, measured in arbitrary consistent length units. This results in the domain length $L_1 = 18$ and width $L_2 = 8$. Constant heads $H_L = 10$ and $H_R = 0$ are prescribed deterministically on the left and right sides of the domain (Figure 1). No-flow boundary conditions are imposed along the lateral boundaries. Locations of 16 points with the known (experimentally determined) hydraulic conductivity values, which are used in conditioning, are shown on Figure 1. In our Monte Carlo and GCOSIM simulations, we assumed that, in the absence of conditioning, the log hydraulic conductivity field $Y(\mathbf{x})$ is statistically homogeneous and isotropic with autocovariance $C_Y(r) = \sigma_Y^2 e^{-r/\lambda}$, where r is separation distance, σ_Y^2 is the variance of $Y(\mathbf{x})$ and λ is its autocorrelation scale. In all examples here presented we assume $\sigma_Y^2 = 1$ and $\lambda = 1$.

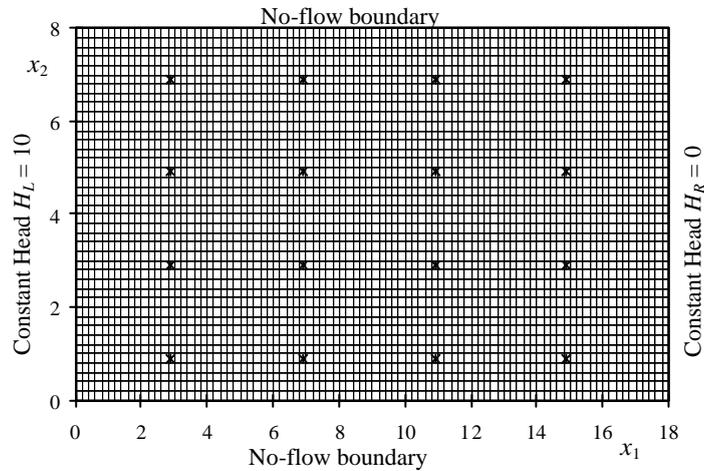


Figure 1. Outline of computational grid and spatial location of Y conditioning points (*).

Figure 2 shows images and longitudinal and transverse cross-sections of conditional mean $\langle Y(\mathbf{x}) \rangle_c$ obtained by *NMC* Monte Carlo realizations and by kriging. To analyze flow by conditional Monte Carlo (MC) simulations, we assign to each element a constant Y value corresponding to the point value generated at its center by GCOSIM. It is seen that values of $\langle Y(\mathbf{x}) \rangle_c$ in the left portion of the domain are generally higher when estimated by kriging procedure than ensemble statistics. Values of $\langle Y(\mathbf{x}) \rangle_c$ computed at locations $10.9 < x_1 < 14.9$ are generally lower when kriging estimates rather than ensemble

moments are employed. This is directly related to the spatial pattern and local values of the “measured” logconductivities.

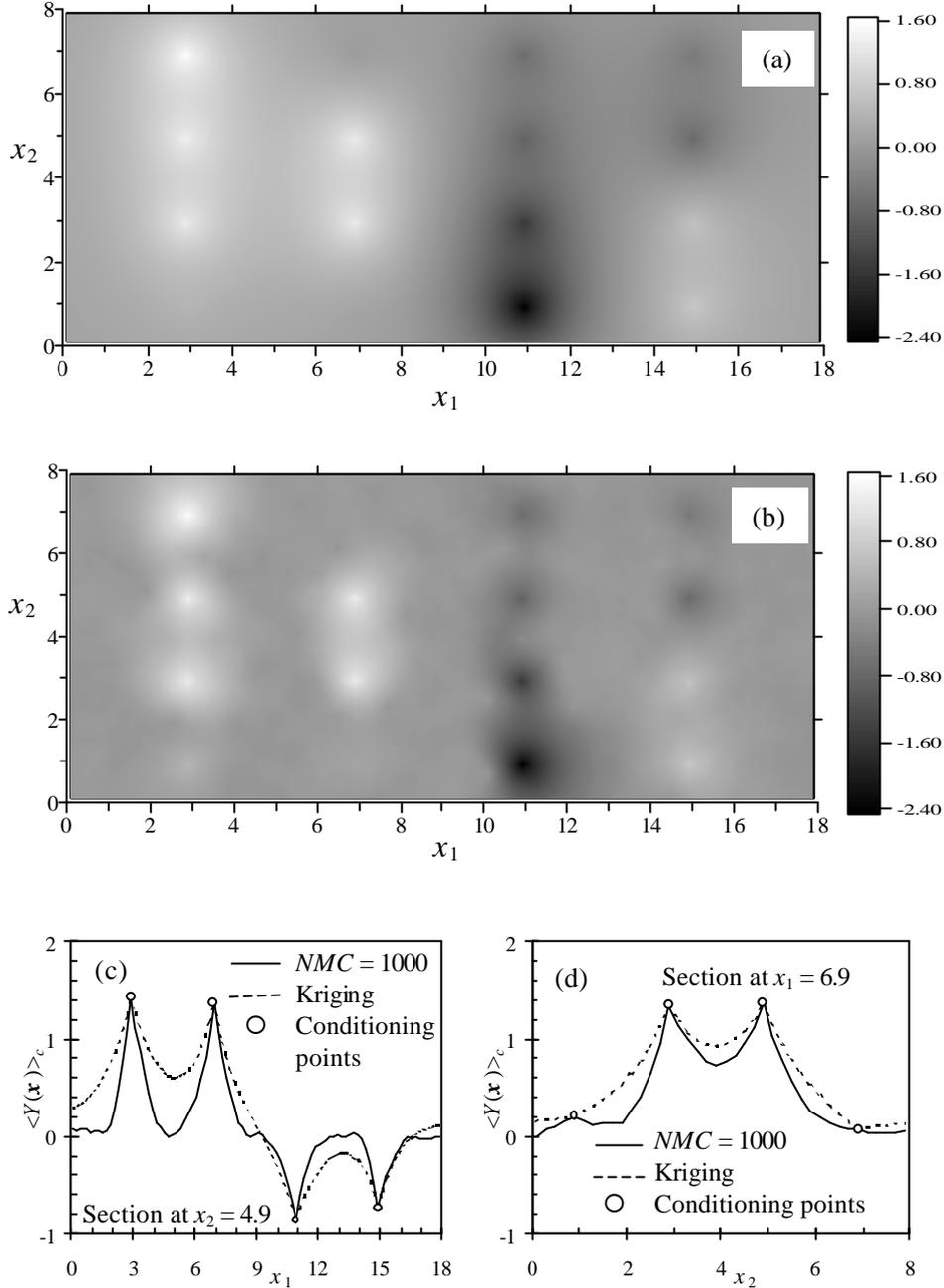


Figure 2. Images of conditional mean $\langle Y(\mathbf{x}) \rangle_c$ field obtained by (a) kriging estimate of actual Y values and (b) $NMC = 1000$ for unconditional $\sigma_Y^2 = 1$, $\lambda = 1$. Sections of $\langle Y(\mathbf{x}) \rangle_c$ at (c) $x_2 = 4.9$ and (d) $x_1 = 6.9$.

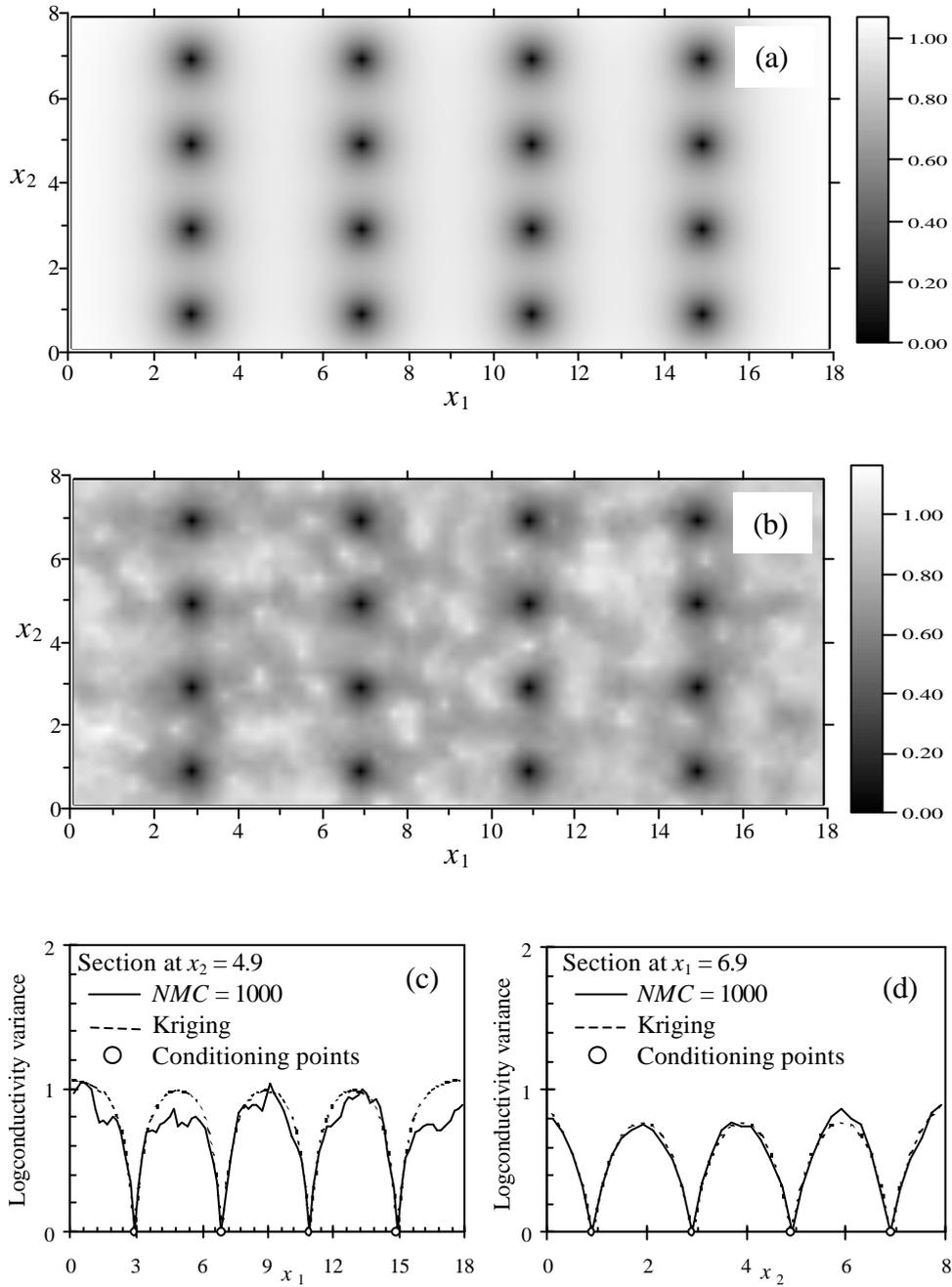


Figure 3. Images of conditional $\sigma_Y^2(\mathbf{x})$ field obtained by (a) kriging equations and (b) $NMC = 1000$ for unconditional $\sigma_Y^2 = 1, \lambda = 1$. Sections of $\sigma_Y^2(\mathbf{x})$ at (c) $x_2 = 4.9$ and (d) $x_1 = 6.9$.

Figure 3 shows images and cross-sections of conditional variance of Y , $\sigma_Y^2(\mathbf{x})$, computed by the two adopted methodologies, showing a satisfactory comparison from a qualitative standpoint. Conditional variance of Y behaves more smoothly and is close to 1 in a larger portion of the field when computed by kriging equations.

Figure 4 depicts mean head $\langle h(\mathbf{x}) \rangle_c$ computed by the three methodologies along a longitudinal section, together with $\langle Y(\mathbf{x}) \rangle_c$ as obtained by ensemble MC and kriging estimate of Y moments. MC and nonlocal results obtained on the basis of ensemble Y fields are virtually indistinguishable. Mean heads $\langle h(\mathbf{x}) \rangle_c$ computed on the basis of the kriged $\langle Y(\mathbf{x}) \rangle_c$ are larger in the left portion of the field, where gradients are flatter.

Figure 5 shows values of longitudinal (parallel to x_1) and transverse (parallel to x_2) component of mean flux obtained by the three methods when $\sigma_Y^2 = 1, \lambda = 1$. Monte Carlo and nonlocal mean fluxes obtained on the basis of ensemble Y fields are virtually indistinguishable; mean fluxes obtained by solving nonlocal equations by using kriging estimates of Y moments capture the general trend but are not able to reproduce the local asperities of the numerical MC solution.

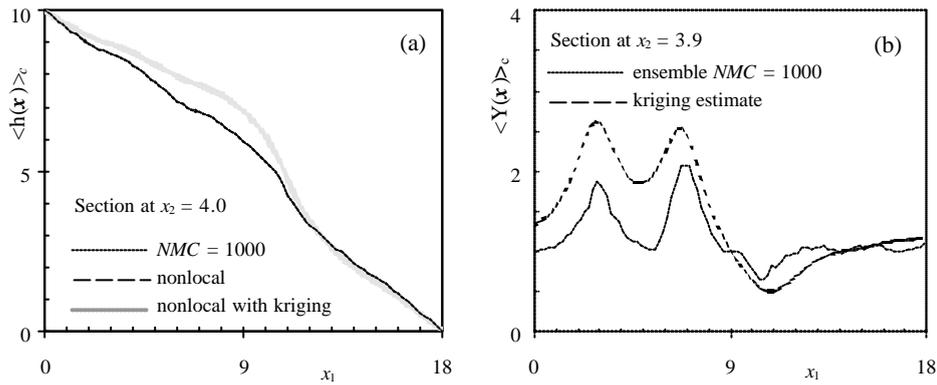


Figure 4. Conditional mean (a) head $\langle h(\mathbf{x}) \rangle_c$ and (b) $\langle Y(\mathbf{x}) \rangle_c$ for unconditional $\sigma_Y^2 = 1, \lambda = 1$.

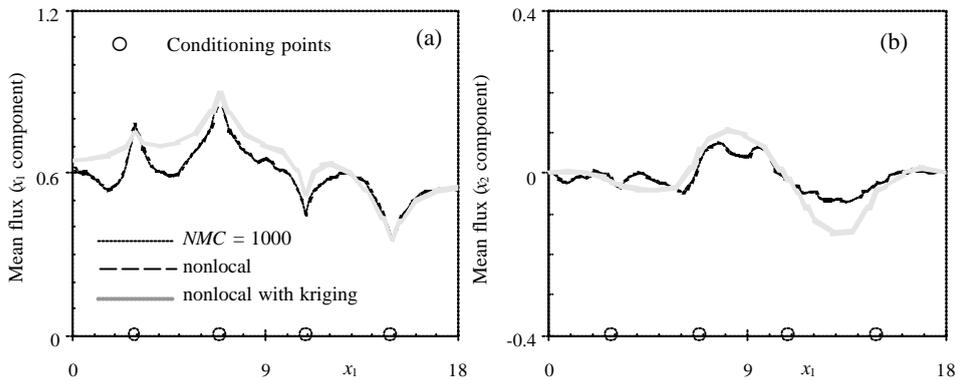


Figure 5. (a) Longitudinal and (b) transverse conditional mean flux along section at $x_2 = 4.9$ (unconditional $\sigma_Y^2 = 1, \lambda = 1$).

Figure 6 depicts values of conditional head variance along the longitudinal cross-sections at $x_2 = 3$, which passes through nodes which share conditioning blocks. Even though our nonlocal results represent the lowest possible order of approximation of the second moments, these compare extremely well with the Monte Carlo results when compatibility between conditional moments of Y in the MC and nonlocal flow solutions is granted, by employing in the latter conditional moments of Y generated by GCOSIM. In this example, the nonlocal solution based on kriged Y fields tends to overestimate the head variance especially close to the lowest $\langle Y(\mathbf{x}) \rangle_c$ values. The same is true about the conditional covariance of head.

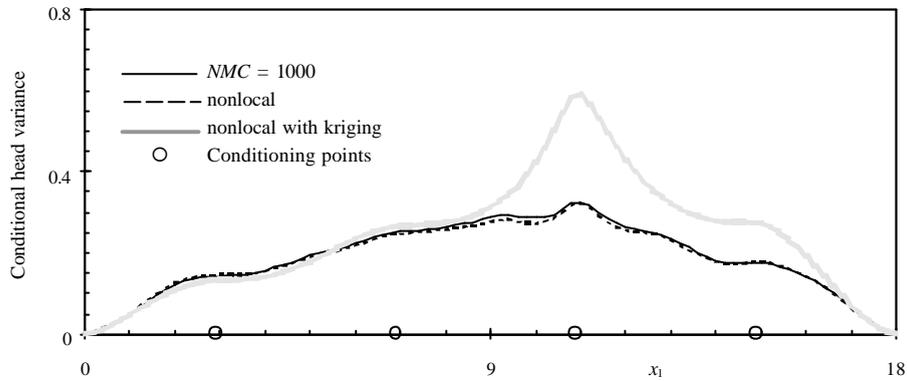


Figure 6. Conditional head variance obtained via MC ($NMC = 1000$; solid), nonlocal finite elements with ensemble estimate of Y moments (dashed) and nonlocal finite elements with kriging estimate of Y moments (gray). Longitudinal section at $x_2 = 3$, unconditional $\sigma_Y^2 = 1$, $\lambda = 1$.

Figure 7 shows how this function varies along the central longitudinal section when the reference point is at the center of the domain ($y_1 = 9, y_2 = 4$).

Figure 8 shows how the components of the flux covariance tensor vary with longitudinal separation distance r_1 from the reference point ($y_1 = 8.9, y_2 = 3.9$).

Figure 9 shows how the conditional variance (covariance at zero lag) of longitudinal and transverse flux, $C_{qc11}(0)$ and $C_{qc22}(0)$, and the cross-covariance $C_{qc12}(0) \equiv C_{qc21}(0)$ between longitudinal and transverse fluxes, vary along a section, which passes through Y -conditioned blocks. Agreement between the first two solutions is excellent; the nonlocal finite element solution obtained by using kriged estimate of statistics of $Y(\mathbf{x})$ varies more smoothly over space but captures the general spatial trend of the different quantities. The variance of longitudinal flux component is generally larger than that of the transverse flux component. The proximity of boundaries causes the variance of transverse flux component to decrease toward zero. Proximity to conditioning points causes the longitudinal variance to dip sharply without necessarily vanishing. Whereas the transverse variance also tends to diminish (albeit slightly and not consistently) at conditioning points, the latter has much lesser impact on the off-diagonal term. The off-diagonal term oscillates uniformly about or near zero in the domain.

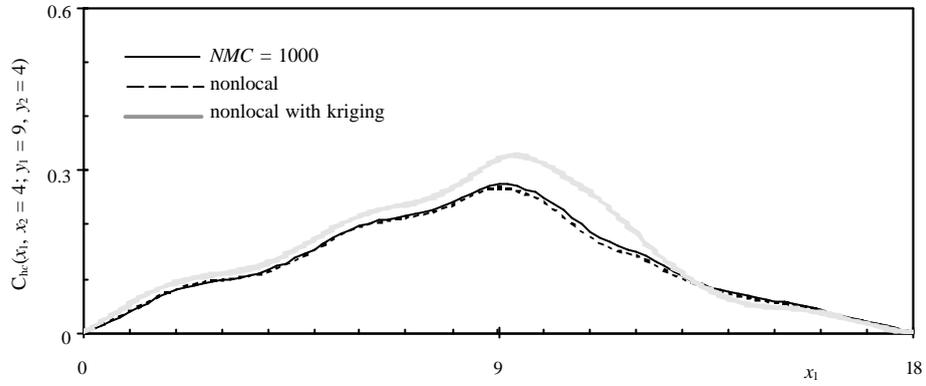


Figure 7. Conditional head covariance $C_{hc}(\mathbf{x}; y_1 = 9, y_2 = 4)$ obtained via MC ($NMC = 1000$; solid), nonlocal finite elements with ensemble estimate of Y moments (dashed) and nonlocal finite elements with kriging estimate of Y moments (gray). Longitudinal section at $x_2 = 4.0$; unconditional $\sigma_Y^2 = 1, \lambda = 1$.

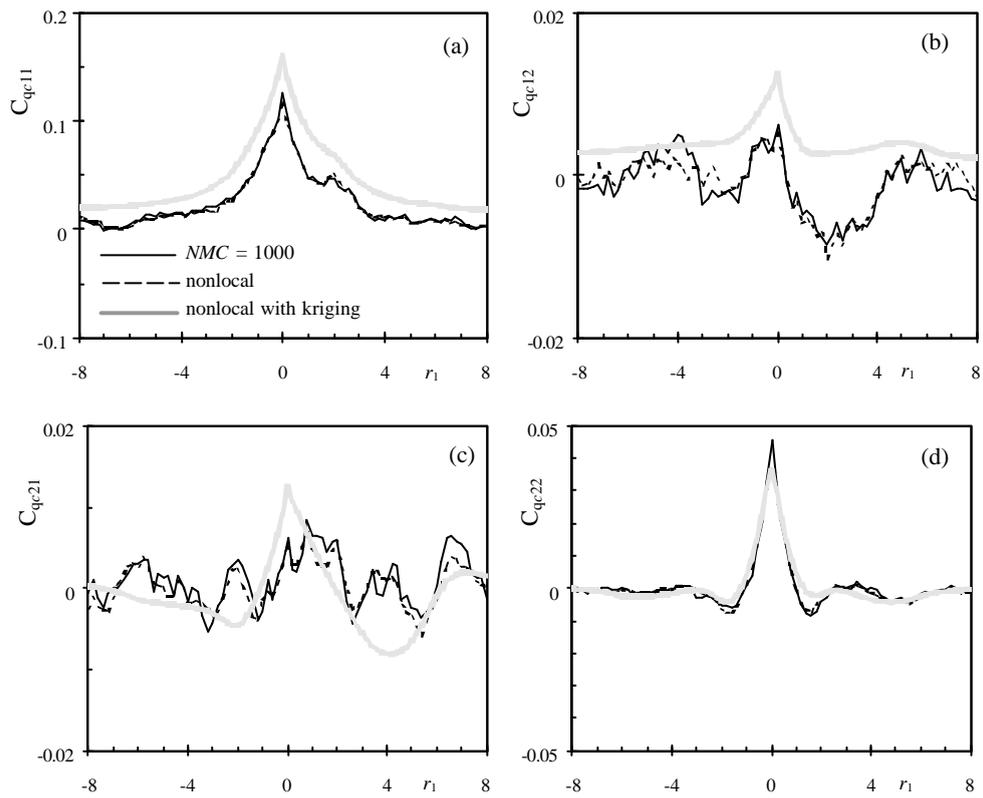


Figure 8. Flux covariance with reference to $y_1 = 8.9, y_2 = 3.9$ as obtained via MC ($NMC = 1000$; solid), nonlocal finite elements with ensemble estimate of Y moments (dashed) and nonlocal finite elements with kriging estimate of Y moments (gray) along a longitudinal section at $x_2 = 3.9$ (unconditional $\sigma_Y^2 = 1, \lambda = 1$).

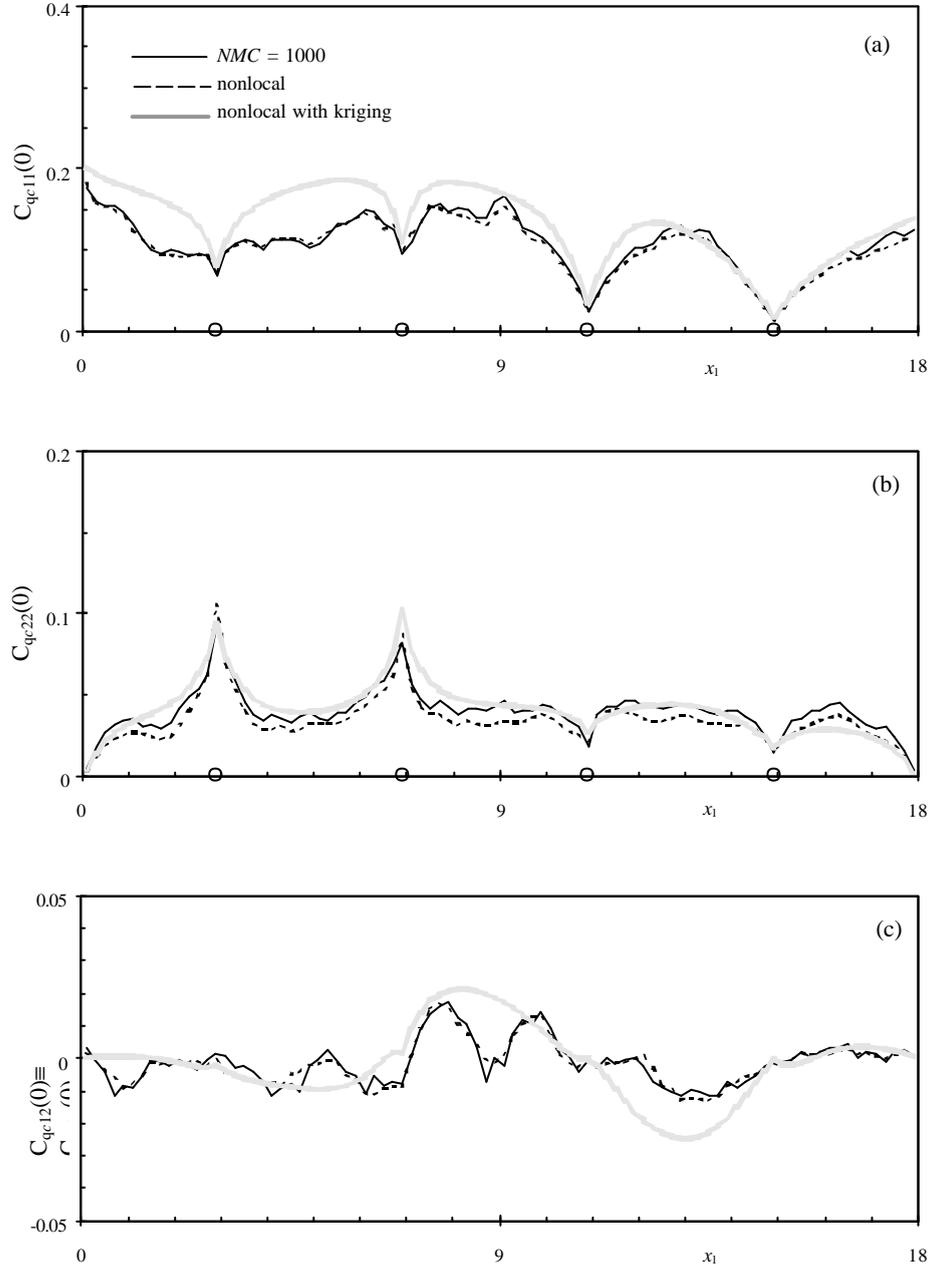


Figure 9. (a) Longitudinal $C_{qc11}(0)$, (b) transverse $C_{qc22}(0)$ flux variance, and (c) cross-covariance $C_{qc12}(0) \equiv C_{qc21}(0)$ between longitudinal and transverse obtained via MC ($NMC = 1000$; solid), nonlocal finite elements with ensemble estimate of Y moments (dashed) and nonlocal finite elements with kriging estimate of Y moments (gray). Longitudinal sections at $x_2 = 4.9$; unconditional $\sigma_Y^2 = 1$, $\lambda = 1$.

4. Conclusions

Our work leads to the following major conclusions:

1. It is possible to render optimum unbiased predictions (and associated prediction errors) of steady state groundwater flow in randomly heterogeneous media under the action of uncertain boundary and source terms deterministically by means of a nonlocal finite element method. The latter is based on a closure approximation of otherwise exact conditional first and second moment equations of flow, and is nominally restricted to mildly heterogeneous media with $\sigma_Y \ll 1$.
2. Our theory assumes that we have at our disposal an unbiased estimate of the hydraulic conductivity $K(\mathbf{x})$, together with the second conditional moment of associated estimation errors. When we compare our nonlocal finite element solution for two dimensional steady state flows with conditional Monte Carlo finite element simulations, we find that the former is highly accurate for $\sigma_Y = 1$, when compatibility between conditional moments of Y in the MC and nonlocal flow solutions is observed. Nonlocal finite element solution obtained by using kriging estimates of moments $Y(\mathbf{x})$ varies more smoothly over space but captures the general spatial trend of estimated heads and fluxes as well as their spatial covariance structure. Since conditional mean quantities are smooth relative to their random counterparts our method allows, in principle, resolving them on relatively coarse grids without upscaling. This feature has not yet been explored.

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